

We Claim:

1. A system for demonstrating signal cascades that occur in certain cells when certain stimuli are introduced, comprising:

- (a) a database of known cellular components and reactions; and
(b) an inference engine for generating signal cascades,

wherein the inference engine is linked to the database.

2. The system of claim 1, wherein the database comprises concepts, events and attributes.

3. The system of claim 2, wherein said concepts are adapted to inherit from other concepts.

4. The system of claim 2, wherein said concepts contain other concepts.

5. The system of claim 2, wherein said concepts exclude other concepts.

6. The system of claim 2, wherein said concepts are capable of joining other concepts.

7. The system of claim 2, wherein said concepts are associated with said attributes.

8. The system of claim 2, wherein said attributes comprise indicia of shape, color, location of a graphic, time, or species.

9. The system of claim 2, wherein said database comprises signal transduction information.

10. The system of claim 2, wherein said database comprises pathology information.

11. The system of claim 2,, wherein said database comprises information specific to chemical areas.

12. The system of 11, wherein said information comprises signal transduction information on plant cellular environments or animal cellular environments.

5 13. The system of claim 1, wherein the database comprises data for binding constants, rate equations, reactant concentrations, primary sequences of functional sites in biomolecules or proteins, or efficacy of physical interactions with binding partners.

14. A computer-implemented method for a reverse pathway comprising:

- 10 (a) providing information regarding a target cellular environment and an endpoint;
- (b) simulating at least one aspect of a reverse pathway based on the information provided regarding the target cellular environment and the endpoint; and
- (c) displaying at least one aspect of the reverse pathway.

15. A computer-implemented method of predicting pathways comprising:

- 15 (a) simulating signal cascades of pathways that occur when stimuli are introduced;
- (b) dynamically generating results using a simulation module, the simulation module comprising an inference engine linked to at least one dynamic database, the at least one dynamic database containing definitions relating to cellular
- 20 concepts, components and reactions.

16. A computer-implemented method for simulating at least one aspect of a cellular biochemical pathway comprising:

(a) providing information regarding a target cellular environment and a stimulus event;

(b) simulating at least one aspect of a cellular biochemical pathway based on the information provided regarding the target cellular environment and the stimulus event; and

(c) displaying at least one aspect of the cellular biochemical pathway.

17. The method of claim 16, wherein the step of displaying further comprises textually or graphically displaying at least one aspect of the cellular biochemical pathway.

18. The method of claim 16, wherein the method further comprises predicting target biological outcomes.

19. The method of claim 16, wherein the method further comprises predicting potential target protein interaction partners.

20. A system for simulating at least one aspect of a cellular biochemical pathway comprising:

(a) a data input interface for receiving cellular environment information and stimuli information;

(b) a simulation module that generates at least one simulated pathway for at least one aspect of a cellular pathway by determining an order of cellular events that occur within a defined cellular environment, wherein the simulation is based on the cellular environment and stimuli information received by the data input interface; and

(c) a display module that displays a representation of the at least one simulated pathway.

21. The system of claim 20, wherein the representation comprises a textual representation.
22. The system of claim 20, wherein the representation comprises a graphical representation.
- 5 23. The system of claim 20, further comprising a prediction module.
24. The system of claim 23, wherein the prediction module predicts at least one biological outcome based on the at least one simulated pathway.
25. The system of claim 24, wherein the at least one biological outcome comprises apoptosis or lymphocyte activation.
- 10 26. The system of claim 23, wherein the prediction module predicts at least one protein interaction partner based upon the at least one simulated pathway.
27. The system of claim 23, wherein the prediction module predicts at least one gene interaction site based upon the at least one simulated pathway.
28. The system of claim 27, wherein the at least one gene interaction site is for
15 transcription factors.
29. A method for generating a representation of a biochemical pathway, comprising:
providing as inputs:
- (a) a set of separately defined concepts and events,
 - (b) a physiological context of the biochemical pathway,

- (c) at least one stimulus, and
- (d) an event corresponding to the at least one stimulus; and

dynamically determining substances available to the biochemical pathway and an order in which events occur in the biochemical pathway.

5 30. The method of claim 29, wherein the separately defined concepts may be associated with various attributes.

31. The method of claim 30, wherein the various attributes comprise information on shape, color, size or location of a graphic.

32. The method of claim 29, wherein at least one of the defined concepts comprises
10 a contextual structure.

33. The method of claim 29, wherein at least one of the defined concepts is a compartment within a cell, part or all of an organelle, a cellular membrane, a cytoskeletal structure, a cell, an extracellular fluid, an extracellular structure, a tissue, an organ, or a compartment within an organ.

15 34. The method of claim 29, wherein
at least one of the defined events may be associated with at least one attribute.

35. The method of claim 34, wherein the at least one attribute comprises reactants, products, inhibitors, and a context within which the at least one of the defined events may occur.

36. The method of claim 34, wherein the at least one attribute comprises information that the at least one of the defined events is inhibited by at least one inhibitor or is inhibited from occurring in at least one location.

37. The method of claim 29, wherein the biochemical pathway comprises a signal
5 transduction pathway.

38. The method of claim 29, wherein the biochemical pathway effects catabolism, anabolism, regulation of oxidative metabolism, regulation of transcription, regulation of protein synthesis, regulation of cell differentiation, or regulation of cell division.

39. The method of claim 29, wherein the biochemical pathway is characteristic of a
10 disease.

40. The method of claim 29, further comprising displaying a representation of at least part of the biochemical pathway.

41. The method of claim 40,
wherein the representation comprises a textual description of objects and
15 processes of at least part of the biochemical pathway, listed in an order in which the objects and processes occur in the pathway.

42. The method of claim 40,
wherein the representation comprises a textual description of objects and
processes of at least part of the biochemical pathway, listed in an order in which the
20 objects and processes occur in order of time step.

43. The method of claim 40, wherein the representation comprises a graphical representation of objects and processes of at least part of the biochemical pathway, wherein at least one of the objects is represented by a graphic symbol having a combination of color, shape, and size unique for the at least one object.

5 44. The method of claim 43, further comprising displaying at least one textual label that identifies the at least one object that is represented by the graphic symbol.

45. The method of claim 43, further comprising displaying at least one textual label that identifies at least one of the processes.

46. The method of claim 43, further comprising displaying a static graphical
 10 representation of part or all the biochemical pathway.

47. The method of claim 43, further comprising displaying a dynamic animated graphical representation of part or all of the biochemical pathway.

48. A method for generating a representation of an event of a biochemical pathway comprising, providing as inputs:

- 15 (a) a set of separately defined reactants of the event,
 (b) a physiological context of the event, and
 (c) at least one defined substance that is a stimulus of the event; and
 dynamically determining an event of the biochemical pathway, comprising a process that is an immediate result of the stimulus.

20 49. The method of claim 48, wherein the process that is an immediate result of the stimulus is a reaction in which at least one reactant of the biochemical pathway reacts and from which at least one product or process of the biochemical pathway is produced.

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50. The method of claim 48, wherein the event of the biochemical pathway is dynamically determined with an inference engine.

51. A method of determining an effect that modulating one or more reactions in a biochemical pathway has on an operation of the biochemical pathway, comprising:

5 (a) generating and displaying a representation of a first biochemical pathway by dynamically determining substances and processes that form the first biochemical pathway, and an order in which the substances appear and the processes occur in the first biochemical pathway;

10 (b) generating and displaying a representation of a second biochemical pathway, wherein a definition of at least one substance or process of the first biochemical pathway is changed so as to modulate at least one reaction of the first biochemical pathway; and

15 (c) comparing the representations of the first and second biochemical pathways and determining an effect of modulating the at least one reaction of the first biochemical pathway.

52. A method of identifying a potential pharmacological target in a biochemical pathway that affects a physiological condition of an organism, comprising:

20 (a) generating and displaying a representation of a first biochemical pathway by dynamically determining substances and processes that form the first biochemical pathway, and an order in which the substances appear and the processes occur in the first biochemical pathway;

(b) generating and displaying a representation of a second biochemical pathway wherein a definition of at least one substance or process of the first biochemical

pathway is changed so as to modulate at least one reaction of the first biochemical pathway; and

- (c) comparing the representations of the first and second biochemical pathways and determining an effect of modulating the at least one reaction of the first biochemical pathway;

wherein a substance of the first biochemical pathway is a potential target for a drug that modulates the reactivity when the substance participates in a reaction which, when modulated, alters the biochemical pathway in a desired manner.

53. A device for generating a representation of a biochemical pathway, comprising:

- (a) means for entering data;
- (b) an electronic storage media that stores definitions of substances and processes of the biochemical pathway;
- (c) a data processing unit that generates a representation of the biochemical pathway; and
- (d) means for displaying a representation of at least one substance or process of the biochemical pathway;

wherein the definitions of each substance and process comprises at least one attribute of the substance or process.

54. A device for generating a representation of a biochemical pathway event, comprising:

- (a) a device for entering input data;
- (b) an electronic storage media that stores definitions of substances and processes from which the biochemical pathway is formed;

(c) a data processing unit that, in response to inputs comprising at least one defined substance or process that is a stimulus of the biochemical pathway event, dynamically determines the biochemical pathway event by determining a process that is an immediate result of the stimulus substance or process; and

5 (d) a display device that displays a representation of at least one substance or process of the biochemical pathway;

wherein the definitions of each substance and process comprises at least one attribute of the substance or process.

55. The device of claim 54, wherein the process that is an immediate result of the
10 stimulus is a reaction in which at least one substance of the biochemical pathway reacts and from which at least one product or process of the biochemical pathway is produced.

56. A device for generating a representation of a pathway, comprising:

- 15 (a) means for entering data;
- (b) means for storing definitions of concepts and events of the pathway;
- (c) means for generating a representation of the pathway; and
- (d) means for displaying a representation of at least one concept or event of the pathway;

wherein the definitions of each concept and event comprises at least one attribute of the concept or event.